

AN ACCURATE QUADRATURE RULE ON THE SPHERE FOR FAST COMPUTATION OF THE RADIATIVE TRANSPORT EQUATION

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ABSTRACT. We present an accurate quadrature formula on the sphere with less localized quadrature points for efficient numerical computation of the radiative transport equation (RTE) in the three dimensions. High accuracy of the present method dramatically reduces computational resources and fast computation of 3D RTE is achieved.

1. INTRODUCTION

We consider an approximation of quadrature on the unit surface,

$$Q(f) = \int_{S^2} f(\xi) d\sigma_\xi \approx Q_K(f) = \sum_{k=1}^K w_k f(\theta_k, \phi_k),$$

where f is a continuous function on S^2 , $d\sigma_\xi$ is the surface element, and $\xi_k = (\theta_k, \phi_k)$ is the standard polar coordinate on S^2 .

One of its application is fast numerical computation of the radiative transport equation (RTE) in the three dimensions which is a mathematical model of near infrared light propagation in human bodies [2, 11]. In brain science, detecting NIR light absorption by hemoglobin is expected to be a new modality for non-invasive monitoring of our brain activities.

Let Ω be a bounded domain with piecewise smooth boundary. We consider the following boundary value problem of RTE

$$(1.1a) \quad -\xi \cdot \nabla_x I - (\mu_s + \mu_a)I + \mu_s \int_{S^2} p(\xi, \xi') I(x, \xi') d\sigma_{\xi'} = q, \quad \text{in } \Omega \times S^2,$$

$$(1.1b) \quad I(x, \xi) = I_1(x, \xi), \quad \text{on } \Gamma_-,$$

where $I = I(x, \xi)$ is light intensity at a position $x \in \Omega \subset \mathbb{R}^3$ with a direction $\xi \in S^2$. The function I_1 is given on $\Gamma_- = \{(x, \xi) ; x \in \partial\Omega, n(x) \cdot \xi < 0\}$, where $n(x)$ is the outer unit normal vector to $\partial\Omega$. The coefficients μ_a and μ_s represent absorption and scattering respectively, and $p(\xi, \xi')$ is called a scattering phase function which represents a conditional probability of a photon changing its velocity from ξ' to ξ by a collision with a scatterer.

Discretizing $\nabla_x I$ by finite difference and scattering integral by a numerical quadrature rule, a system of linear algebraic equations is obtained [7]. Since (1.1) in the spatial three dimensions is essentially a five dimensional problem, numerical

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computation requires huge resources (time and storage). And for its unique solvability, errors in the quadrature rule should be sufficiently small [4]. In some examples, computation of the scattering integral spends over 80% of total computational time [5]. This means that a novel treatment of scattering integral is effective for fast computation.

A simple approximation for $Q(f)$ is repeating the trapezoidal rule to both zenith and azimuthal directions as

$$(1.2) \quad Q(f) = \int_0^{2\pi} \int_0^\pi f(\theta, \phi) \sin \theta \, d\theta \, d\phi \approx \frac{\pi}{M_\theta} \frac{2\pi}{M_\phi} \sum_{m=0}^{M_\theta} \sum_{n=0}^{M_\phi-1} f(\theta_m, \phi_n) \sin \theta_m,$$

where $\theta_m = m\pi/M_\theta$ and $\phi_n = 2n\pi/M_\phi$. This is convenient in application since both the weights and the nodes (θ_m, ϕ_n) are explicitly known. However a large number of nodes should be taken due to its low accuracy. Moreover, they localize near the poles and associated weights are small relatively. This indicates that unknowns near the poles formally introduced in discretization have less meaning.

2. A NEW QUADRATURE RULE ON THE SPHERE

We construct high-accurate quadrature rule on the sphere with less localized quadrature points to reduce a number of discretization points for the velocity direction $\xi \in S^2$ in (1.1a).

To state more precisely, we introduce some basic concepts from [10]. For a linear subspace $V \subset C(S^2)$, we say Q_K is *exact* on V if $Q_K(f) = Q(f)$ for any function $f \in V$. For a finite rotation group $G \subset SO(3)$, Q_K is said to be *invariant* under G if the set of quadrature points $\{\xi_k\}$ is a disjoint union of G -orbits, $\{\xi_k\} = \{g\xi'_1; g \in G\} \cup \dots \cup \{g\xi'_s; g \in G\}$, and $w_k = w_j$ if ξ_k and ξ_j belong to the same orbit. For $f \in V$ and $g \in G$, we set $f_g(x) = f(gx)$ and $V_G = \{f \in V; f_g = f \text{ for any } g \in G\}$.

For high-accuracy of Q_K , we require that it is exact on

$$\Pi^N = \text{span}\{Y_n^m; |m| \leq n \leq N\}$$

for some non-negative integer N , where

$$Y_n^m(\theta, \phi) = (-1)^m \sqrt{\frac{2n+1}{4\pi} \frac{(n-m)!}{(n+m)!}} P_n^m(\cos \theta) e^{im\phi}, \quad |m| \leq n,$$

is a spherical harmonic of degree n and order m [1]. The functions $\{Y_n^m; |m| \leq n\}$ form a complete orthogonal system of $L^2(S^2)$ with

$$Q(Y_n^m) = \sqrt{4\pi} \delta_{n0} \delta_{m0},$$

thus Q_K satisfies

$$(2.1) \quad Q_K(Y_n^m) = \sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = \sqrt{4\pi} \delta_{n0} \delta_{m0}, \quad \text{for any } |m| \leq n \leq N.$$

Exactness on Π^N is motivated by the spherical harmonic expansion of an analytic function f on S^2 ,

$$f(\theta, \phi) = \sum_{n=0}^{\infty} \sum_{|m| \leq n} a_{nm} Y_n^m(\theta, \phi)$$

where coefficients $|a_{nm}|$ decrease exponentially with respect to n [9]. Hence the error $|Q_K(f) - Q(f)|$ decays rapidly with respect to N .

For less localized distribution of quadrature points, we require that Q_K is also rotationally invariant under the icosahedral group. Hence we call the proposed approximation *RIQS20* (Rotationally Invariant Quadrature rule on the Sphere under the icosahedral group).

If Q_K is invariant under some finite rotation group G and exact on Π_G^N , then it is exact on Π^N [8]. Therefore (2.1) for all $|m| \leq n \leq N$ are redundant. The next theorem gives an example of reduction of (2.1) using symmetries of Y_n^m . It also reduces (2.1) to real-valued equations.

Theorem 2.1. *Suppose that $\{w_k, \theta_k, \phi_k\}$ in Q_K satisfies the following conditions: (i) for any (θ_k, ϕ_k) , there uniquely exists (θ_j, ϕ_j) such that $(\theta_j, \phi_j) = (\theta_k, \phi_k + \pi)$ and $w_j = w_k$, and (ii) for any (θ_k, ϕ_k) , there uniquely exists (θ_j, ϕ_j) such that $(\theta_j, \phi_j) = (\theta_k + \pi, \pi - \phi_k)$ and $w_j = w_k$. Then, the system (2.1) is equivalent to*

$$(2.2a) \quad \operatorname{Re} \sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = \sqrt{4\pi} \delta_{n0} \delta_{m0}, \quad \text{if } n \text{ is even or } 0,$$

$$(2.2b) \quad \operatorname{Im} \sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = 0, \quad \text{if } n \text{ is odd},$$

for any $(m, n) \in \{(2\mu, 2\nu); 0 \leq 2\mu \leq 2\nu \leq N, \mu, \nu \in \mathbb{Z}\} \cup \{(2\mu, 2\nu + 1); 0 < 2\mu \leq 2\nu + 1 \leq N, \mu, \nu \in \mathbb{Z}\}$.

Proof. Note that Y_n^m satisfies following symmetries,

$$(2.3) \quad Y_n^m(\theta, \phi + \pi) = (-1)^m Y_n^m(\theta, \phi),$$

$$(2.4) \quad Y_n^m(\theta + \pi, \pi - \phi) = (-1)^n \overline{Y_n^m(\theta, \phi)},$$

and

$$(2.5) \quad Y_n^{-m}(\theta + \pi, \pi - \phi) = (-1)^{n+m} Y_n^m(\theta, \phi).$$

From the assumption (i) and (2.3), we have

$$\sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = 0, \quad \text{if } m \text{ is odd.}$$

Similarly, from the assumption (ii) and (2.4), we have

$$\operatorname{Im} \sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = 0, \quad \text{if } n \text{ is even,}$$

$$\operatorname{Re} \sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = 0, \quad \text{if } n \text{ is odd,}$$

and

$$\sum_{k=1}^K w_k Y_n^0(\theta_k, \phi_k) = 0, \quad \text{if } n \text{ is odd.}$$

To sum up, we obtain Table 1 under conditions (i) and (ii). Finally,

$$\sum_{k=1}^K w_k Y_n^m(\theta_k, \phi_k) = 0, \quad m > 0$$

TABLE 1. Real and imaginary parts of $Q_K(Y_n^m)$ under conditions (i) and (ii)

n	m	Real part	Imaginary part
even, 0	even, 0	(2.2a)	0
	odd	0	0
odd	even, $\neq 0$	0	(2.2b)
	odd, 0	0	0

leads

$$\sum_{k=1}^K w_k Y_n^{-m}(\theta_k, \phi_k) = 0, \quad m > 0$$

from the assumption (ii) and (2.5). This concludes the proof. \square

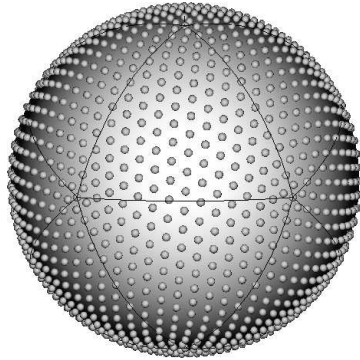
The system of equations (2.2) is solved numerically with the Newton iteration or the homotopy method in this study. In the computation we use a representation of the icosahedral group which does not change the icosahedron with vertices

$$(2.6) \quad (\pm 1, 0, \pm \alpha), \quad (\pm \alpha, \pm 1, 0), \quad (0, \pm \alpha, \pm 1), \quad \alpha = \frac{\sqrt{5} - 1}{2}.$$

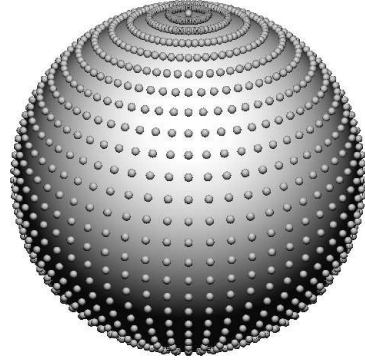
It gives an orbit which satisfies the conditions in Theorem 2.1 [6].

3. NUMERICAL EXAMPLES

Constructed quadrature points of RIQS20 with the degree 75 are shown in Figure 1(a), where solid curves show the projection of the icosahedron (2.6). The number of quadrature points on S^2 is 1932, and they are less localized by virtue of rotational invariance than those of (1.2) shown in Figure 1(b).



(a) RIQS20 (proposed method), degree 75, #Nodes = 1932



(b) Repeating trapezoidal rules (1.2), $M_\theta = 30, M_\phi = 60$, #Nodes = 1742

FIGURE 1. Quadrature points on S^2

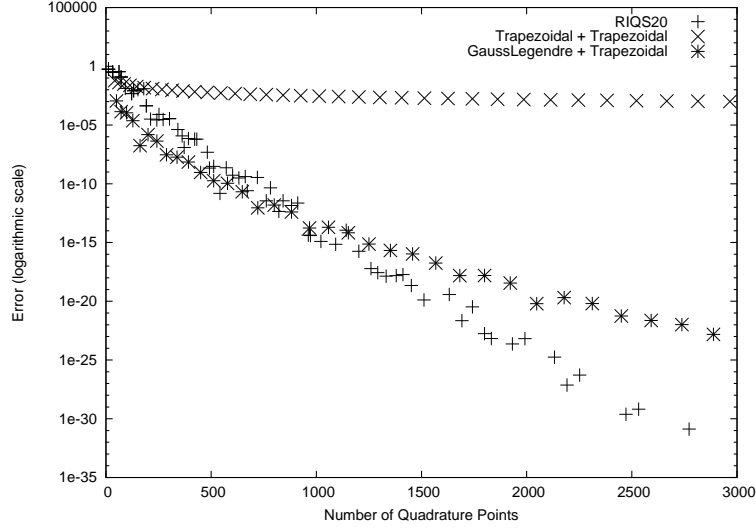


FIGURE 2. Numerical errors

Figure 2 shows the numerical errors $|Q_K(f) - Q(f)|$ for

$$f(\xi) = \frac{1}{4\pi} \frac{1 - g^2}{(1 - 2g\xi \cdot \xi' + g^2)^{3/2}}, \quad \xi' = \left(\frac{1}{9}, \frac{4}{9}, \frac{8}{9}\right), \quad g = \frac{1}{2},$$

which corresponds to $p(\xi, \xi')$ in 3D RTE as a Henyey-Greenstein kernel and satisfies $Q(f) = 1$. In addition to RIQS20 (+ signs) and repeating trapezoidal rules (1.2) (TT; \times signs), the Gauss-Legendre rule (GLT; $*$ signs) to the θ -direction in (1.2) is also examined. The method GLT is expected to be accurate since both the Gauss-Legendre rule and the trapezoidal rule for a periodic function are accurate although it has also the defect in localization of quadrature points. RIQS20 is most accurate among three quadrature rules.

Table 2 shows the maximum and minimum of weights in these three quadrature rule. More precisely, 1920 nodes (99.4%) have weights between 4.4×10^{-3} and 7.0×10^{-3} in RIQS20 with the degree 75. This means that almost all function values on the quadrature points contribute equivalently to numerical quadrature and thus it is reasonable in discretization of unknown function in an integral equation.

TABLE 2. Maximum and minimal weights, the number of nodes associated the weights

Quadrature	Maximum	Minimum
RIQS20, degree 75	6.9938×10^{-3} (60 nodes)	2.5423×10^{-3} (12 nodes)
TT, $M_\theta = M_\phi/2 = 30$	1.0966×10^{-2} (60 nodes)	1.1462×10^{-3} (120 nodes)
GLT, $M_\theta = M_\phi/2 = 30$	1.0771×10^{-2} (120 nodes)	8.3443×10^{-4} (120 nodes)

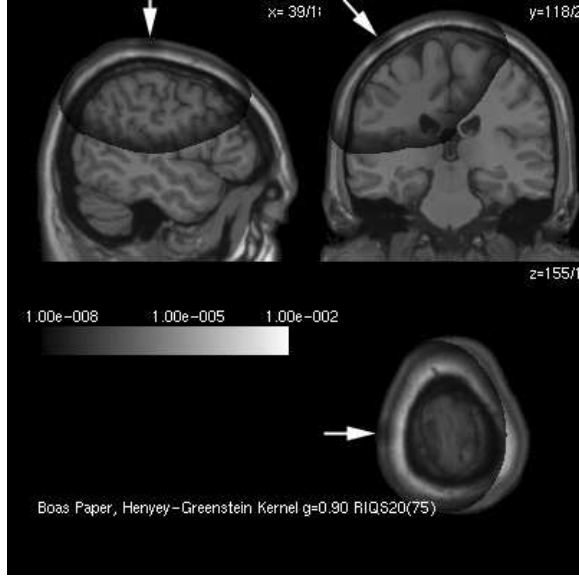


FIGURE 3. Numerical results

4. APPLICATION TO 3D RTE

Finally we show efficiency of RIQS20 in numerical computation of stationary 3D RTE. As a numerical example, we use an MR image of an adult human head which consists of $181 \times 217 \times 181$ voxels (1mm^3 cubes, Figure 3) and 4.1 million special points inside the domain. Optical parameters reported in [3] are adopted. We employ the Gauss-Seidel iteration to solve the linear equation due to its diagonal dominance [4]. The iteration is stopped with 3000 iterations, by which the relative residual is approximately 7×10^{-2} in the maximum norm.

Using the trapezoidal rule (1.2) with $M_\theta = 60$ and $M_\phi = 120$, the number of quadrature points for the velocity direction $\xi \in S^2$ is 7082 and the number of unknowns in the linear system is 28.7 billion, which corresponds to 214 gigabytes in double precision. Computational time is approximately 87.0 hours on Opteron 6238 (2.5GHz) with 1024 MPI processes. On the other hand, using RIQS20 with the degree 75, the number of nodes on S^2 is 1932 and the number of unknowns is 7.8 billion, which corresponds to 58 gigabytes. The computational time on the same environment is reduced to 6.3 hours. Moreover, we can process the computation on 4 PCs (Core i7-4770, 3.4GHz) with GPU (GeForce GTX TITAN) and the computational time is 17.4 hours. The results show that RIQS20 is quite effective in computation of 3D RTE.

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TABLE 3. Computational resources for 3D RTE

Cubature Formula	#Unknowns	Parallelization	Computational Time
Trapezoidal Rule (1.2) $M_\theta = M_\phi/2 = 60$	28.7×10^9 (214 GB)	1024 proc	87.0 hours
RIQS20 (proposed) degree 75	7.8×10^9 (58 GB)	1024 proc 4 PC with GPU	6.3 hours 17.4 hours

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